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ARTIFICIAL INTELLIGENCE IN HERBAL NANO FORMULATION: A COMPREHENSIVE REVIEW

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Abstract: A revolutionary approach to contemporary drug development is the combination of artificial intelligence (AI) and nano-herbal formulation. Conventional herbal remedies frequently have drawbacks such poor bioavailability, inconsistent composition, and a lack of pharmacokinetic knowledge. While AI offers strong tools for data analysis, prediction, and optimisation, nanotechnology enables better phytochemical solubility, stability, and targeted distribution. AI-based deep learning and machine learning models have been used to improve quality control, predict bioactivity, develop appropriate nanocarriers, optimise extraction settings, and evaluate toxicity. These methods promote individualised therapeutic tactics, expedite formulation development, and lessen the workload associated with experiments. While AI- driven optimisation is used, case studies using curcumin, ginseng, and other nano-herbal systems show increased bioavailability and therapeutic efficacy. Notwithstanding its benefits, issues with data accessibility, standardisation, governmental permission, and ethical considerations still exist. All things considered, the combination of AI and nano-herbal technology presents a promising avenue for future pharmaceutical research by offering substantial promise for safer, more effective, and patient-specific treatments.

Keywords: Artificial Intelligence (AI), Machine learning, Extraction, Nano-Herbal formulation, Nano technology, Drug Delivery System, Bioavailability.

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INTRODUCTION

Since many plants have significant medicinal benefits, herbal medicine has been an essential component of traditional healthcare systems for generations. However, elements including low bioavailability, inconsistent composition, and a lack of knowledge about their pharmacological effects can compromise both safety and effectiveness of these herbal remedies. New herbal formulations that increase absorption and medicinal efficacy have become possible due to nanotechnology. AI has emerged as an essential tool in nano-herbal medicine, helping with formulation development optimisation, bioactivity prediction, and the analysis of large datasets. (1) The integration of engineering and scientific study combined the objective of building intelligent machines is known as artificial intelligence. These devices are made to simulate human cognitive processes, particularly learning and problem-solving, utilising algorithms or a set of predetermined rules. AI systems are able to function with intelligence, purpose, and adaptability because they can anticipate possible problems or handle them as they come up . The ability of artificial intelligence to analyse vast amounts of multidimensional, multimodal data and find patterns and relationships within them is what gives it its power. AI systems, for example, can summarise a patient's whole medical history into one consolidated figure that represents an accurate diagnosis. Furthermore, due to AI systems are autonomous and dynamic, they may keep learning and developing as new data becomes available. (2) Rather than being viewed as a single, all-encompassing technology, it is critical to understand that artificial intelligence (AI) is a wide concept embracing various subfields ,encompassing methods like machine learning and deep learning. These subfields enhance intelligence in a range of situations, whether they are applied separately or in conjunction. Specifically, machine learning (ML) focusses on developing algorithms that enable computer systems to self-improve through experience learning. (3)

ARTIFICIAL INTELLIGENCE IN NANO HERBAL EXTRACTION

Artificial intelligence algorithms, particularly those referring to ML and DL, have been utilised in the field of nano-herbal extraction to optimise extraction parameters like as temperature, pressure, solvent composition, and extraction duration. These algorithms are skilled at examining sizable datasets and discovering trends that aid in forecasting the best extraction circumstances for certain herbal extracts. For example, a 25% increase in extraction yield was achieved by improving the ginsenoside extraction conditions from ginseng using a machine learning algorithm. (4).

NANOTECHNOLOGY-BASED DRUG DELIVERY SYSTEM FOR PHYTOCHEMICAL COMPOUNDS

Studies reveal that a significant 70% of plant-derived bioactive

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chemicals are hydrophobic. Utilising the latest innovations has emerged as a tactical approach aimed to boosting bioavailability and bioactivity of phytochemical substances. Creating appropriate drug delivery formulations is crucial to advancing the development of innovative nanotechnology-based therapies. For the prevention and treatment of disease, effective phytochemical delivery is essential. Lipid-based and polymer-based delivery methods are particularly promising for increasing the bioactivity of these phytochemical substances. (5) To guarantee the efficient delivery of herbal medications, sophisticat ed drug delivery systems based on nanotechnology have been created. (6)

TYPE OF DRUG DELIVERY SYSTEM;

1) Lipid based delivery system
2) Polymeric Nano carriers

LIPID BASED DELIVERY SYSTEM;

1) Vesicular system;

- Liposome
- Phytosomes
- Transfersome
- Ethosome
- Niosome

2) Lipid particulate

- Solid-lipid nanoparticle
- Nano structural lipid carrier (NLC)

3) Nano emulsion

POLYMERIC NANO CARRIERS;

- Polymeric nanoparticle
- Dendrimer
- Polymersome
- Miscelles(7)

LIPID BASED DELIVERY SYSTEM;

1) VESICULAR SYSTEM;

• LIPOSOME

One or more phospholipid layers produce the spherical sacs known as liposomes. Both fat- soluble and water-soluble medications can be carried by them (8). By stabilising chemicals, enhancing cellular and tissue absorption, and boosting medication biodistribution to target areas, liposomes are adaptable drug delivery vehicles that improve treatment efficacy (9). They provide focused delivery, low toxicity, excellent biocompatibility, and biodegradability, which set them apart from conventional techniques. Pharmaceuticals, cosmetics, food, and tissue engineering are just a few of the businesses that employ liposomes (10).

• PHYTOSOMES

Phospholipids and plant extracts or phytoconstituents combine to form lipid-compatible molecular complexes in phytosomal formation. Here in the phytosomes, the solubility of poorly water-soluble phytoconstituents may be enhanced. The phospholipids are usually employed in phytosome formation. Phytosome formulation enhances the pharmacokinetic, pharmacodynamic, absorption, and bioavailability characteristics.(11)

• TRANSFERSOME

Transferosomes are vesicular carrier systems with using a suitable edge activator along with at least one inner aqueous compartment surrounded by a lipid bilayer (12). Ultra-deformable vesicles with self-optimizing and self-regulating properties are created by this aqueous core encased in a lipid bilayer (13). Transferosomes are hence stretchy. Through skin pores or constrictions that are much smaller than the vesicle size, they can distort and squeeze themselves as whole vesicles without a discernible loss. (14)

• ETHOSOME

Ethosomes are flexible, soft vesicles mostly made of water, ethanol (at a comparatively high concentration), a phospholipid. These soft vesicles are an example of new vesicular carrier for improved skin delivery. Ethosome vesicles can range in size from tens of microns to nanometres. This carrier has intriguing characteristics relating to its great deformability, which allows it to pass through human skin intact.(15)

• NIOSOME

Niosomes are vesicular systems that are created when nonionic surfactants self-assemble in an aqueous solution with the help of physical agitation or high temperatures. (16) The Many of the drawbacks of liposomes, including inadequate chemical stability, phospholipids' propensity for oxidation, high production costs, the need for special handling, and storage conditions, are overcome by using nonionic surfactants as membrane-forming components in place of phospholipids. (17)

2) LIPID PARTICULATE

• SOLID-LIPID NANOPARTICLE (SLNs)

Since its introduction in the early 1990s, SLNs are acknowledged as an alternative to the traditional colloidal drug carriers, such as liposomes, microemulsions, and microparticles and nano emulsions (18) in place of liquid integration of solid lipids with the lipid of emulsion systems such as fatty acids (stearic acid) and triglycerides (tri-stearin). or palmitic acid), or waxes (cetyl palmitate) to make up lipophilic core to spread or dissolve hydrophobic medications, emulsifiers that stabilise systems, or stabilizing agents in addition to their nanometric size (around solid lipid depression systems in the 40–200 nm range, i.e. SLNs are regarded as first-generation novels. medication carriers made of lipids.(19)

• NANOSTRUCTURED LIPID CARRIER (NLC)

Higher drug loading is made possible by this balanced imperfect nanostructured lipid carriers (NLCs) matrix, which also begins to display characteristics of both Delivery systems include SLNs and emulsions. NLCs are classified into three categories based on the methodology: (1) imperfect type NLCs, which have an imperfect solid structure matrix; (2) amorphous type NLCs, which have a structureless solid amorphous matrix; and (3) multiple type NLCs, which have multiple oil in fat in water, or O/F/W.(20)

3) NANO EMULSION

The term nano emulsion refers to a colloidal dispersion of two thermodynamically unstable immiscible liquids. In nano emulsion, one of the liquids produces the dispersed phase and other liquid forms the dispersion medium .(21) Droplets make up a nano emulsion. Each droplet has a protective layer of emulsifier molecules, and their sizes range from 10 to 200 nm (22).

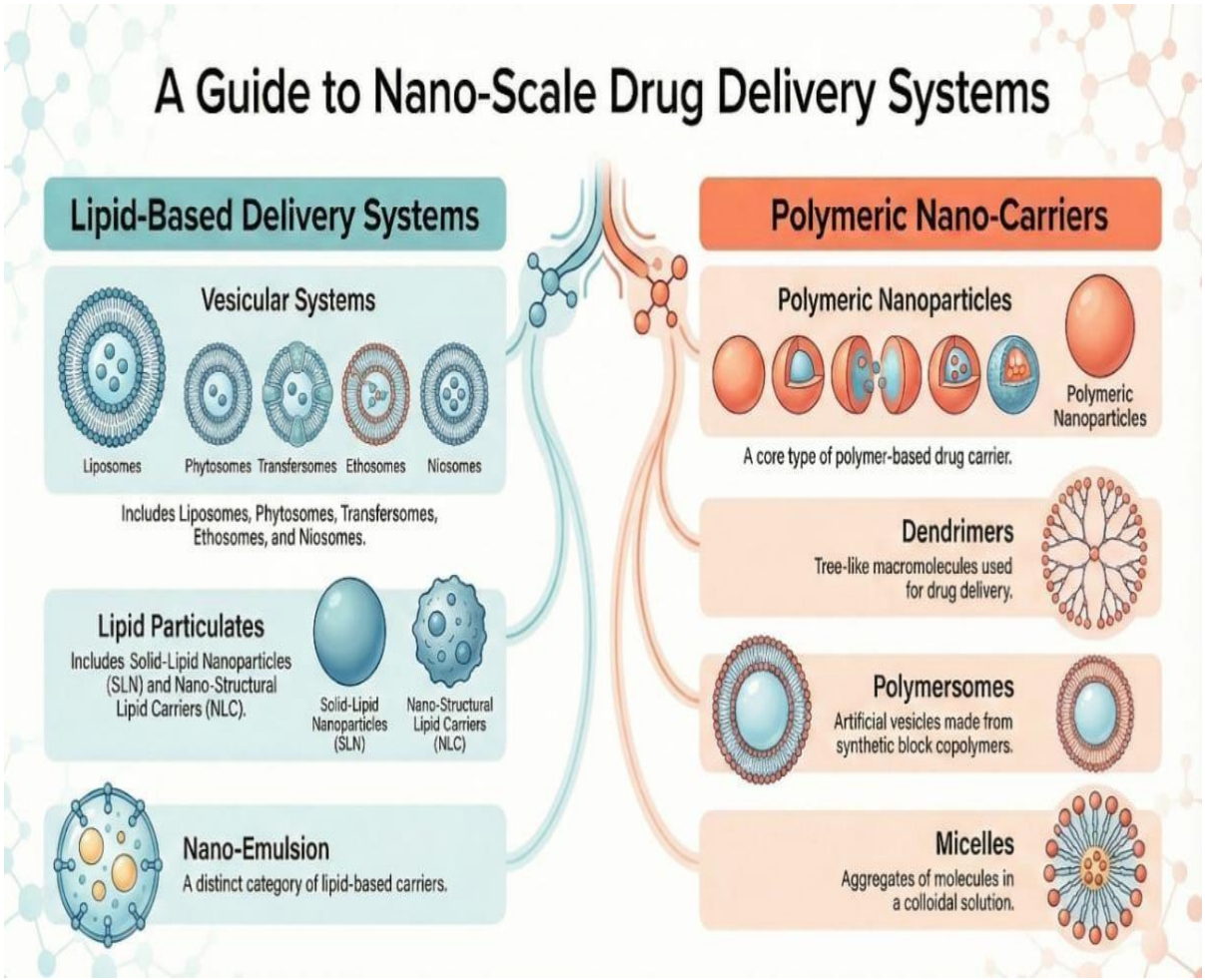

Figure: 1 types of nano drug delivery system

POLYMERIC NANO CARRIERS;

• POLYMERIC NANOPARTICLE

Solid colloidal particles made of biodegradable and biocompatible polymers are known as polymeric nanoparticles (23). They can improve targeted drug delivery by releasing medications in response to different inputs. And effectiveness against cancer (24). Targeted drug delivery systems can benefit from NPs with phosphate ester moieties that are enzymatically degradable because they can alter their zeta potential (25)

• DENDRIMER

Dendrimers are tree-shaped macromolecules with many functional groups on the outside, hollow interiors, and a central core (26). Dendrimers are highly branched macromolecules with special qualities that make them appropriate for biomedical uses such gene therapy, medication transport, and diagnostic imaging (27). They display cytotoxicity and haemolysis, whereas cationic dendrimers have longer circulation durations and less toxicity (28). Because they exhibit less cytotoxicity and haemolysis, dendrimers with carboxylate terminal groups and those grafted with polyethylene oxide are better suited for biological applications. (29) They can improve medication delivery, encapsulate or combine with therapeutic medicines, and shield genetic elements from enzymatic deterioration (30)

• POLYMERSOME

Amphiphilic block copolymers are used to create artificial synthetic structures known as polymersomes or polymeric vesicles. (31) Creating hydrophilic and hydrophobic blocks with the necessary properties (32) permit the addition of hydrophilic molecules to their aqueous core as well as hydrophobic substances to the interior of the membrane of a polymersome (33)

• MICELLES

Proteins including MG2, sIgA, lactoferrin, and lysozyme are encapsulated in micelles, which are self-assembling colloidal structures made of amphiphilic molecules in aqueous solutions. Micelles help to maintain homeostasis in biological systems (34). Numerous methods, including cryo-TEM, dynamic light scattering, small-angle neutron scattering, and fluorescence correlation spectroscopy, which aid in determining the size, structure, and interactions of micelles with biological settings .(35)

MACHINE LEARNING AND DEEP LEARNING FOR THE FORMULATION:

In drug design, deep neural networks (DNNs), especially CNNs and RNNs, are extremely helpful tools. CNNs are particularly good at processing data that resembles images, like 2D or 3D point clouds of molecular structures. (36) Multi-layered neural networks are employed in deep learning, a specialised subset of machine learning, that extracts highly abstract representations from complicated, high-dimensional input. Deep learning models, such as convolutional neural networks (CNNs) and recurrent neural networks (RNNs), are especially well-suited for analysing molecular structures, time-series pharmacokinetic data, and pictures (such as histopathology). Deep learning has demonstrated potential in pharmaceutical research and development for intelligent drug screening, drug-target mapping, and protein-ligand interaction prediction. (37) While transformer-based models process sequential data to predict patient- specific responses, such as in andrographolide formulations, deep learning techniques, such as graph neural networks (GNNs), are increasingly used in nanoemulsion-based drug delivery to capture complex temporal patterns in release kinetics. On the other hand, in order to forecast compatibility based on molecular descriptors, dendrimers and phytosomes have mostly been explored using machine learning models, including support vector machines (SVMs), and various unsupervised clustering techniques, encompassing methods like k-means and principal component analysis (PCA). However, due to the very tiny & less varied training datasets, deep learning applications in these carriers are still restricted. (38,39)

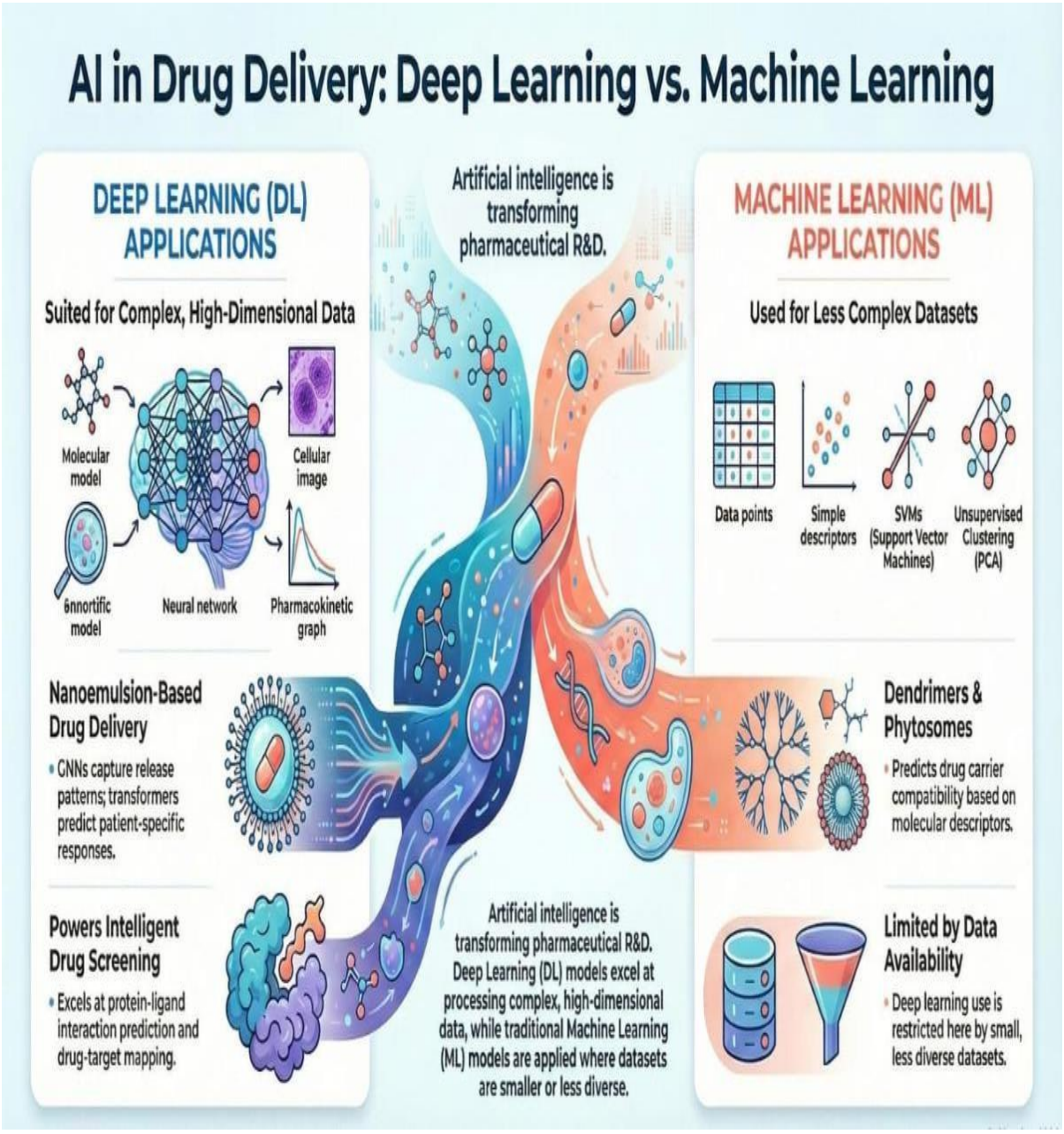
AI in Drug Delivery: Deep Learning vs. Machine Learning
DEEP LEARNING (DL) APPLICATIONS
Suited for Complex, High-Dimensional Data
Molecular model
Cellular image
6nnortific model
Neural network
Pharmacokinetic graph
Artificial intelligence is transforming pharmaceutical R&D.
MACHINE LEARNING (ML) APPLICATIONS
Used for Less Complex Datasets
Data points
Simple descriptors
SVMs (Support Vector Machines)
Unsupervised Clustering (PCA)
Nanoemulsion-Based Drug Delivery
GNNs capture release patterns; transformers predict patient-specific responses.
Dendrimers & Phytosomes
Predicts drug carrier compatibility based on molecular descriptors.
Powers Intelligent Drug Screening
Excels at protein-ligand interaction prediction and drug-target mapping.
Artificial intelligence is transforming pharmaceutical R&D. Deep Learning (DL) models excel at processing complex, high-dimensional data, while traditional Machine Learning (ML) models are applied where datasets are smaller or less diverse.
Limited by Data Availability
Deep learning use is restricted here by small, less diverse datasets.

Figure: 2 AI models in drug formulation

AI NANO HERBAL VACCINES;

When it comes to effectively processing and analysing the chemical structures, biological activities, and pharmacological characteristics of herbal compounds, artificial intelligence algorithms outperform conventional methods. For example, the time and expense associated with drug development can be greatly reduced by using machine learning models to evaluate the chemical fingerprints of nano-formulated herbal compounds in order to predict their efficacy. This method simplifies testing procedures and makes it easier to find candidates for additional development.

EXAMPLES OF NANO HERBAL VACCINES:

The potential of nano-herbal vaccines to cure a diverse array of infectious diseases has been observed the subject of numerous investigations, including:

INFLUENZA:

A liposomal formulation of a nano herbal vaccine, which contains the herbal extract Echinacea purpurea, has been shown to be effective against influenza, as reported in the literature published in the Journal of Controlled Release. (40)

HEPATITIS B:

To develop a nano-herbal vaccination for hepatitis B, researchers have created a polymeric nanoparticle system that contains the herbal ingredient Glycyrrhiza glabra. (41)

MALARIA:

A study that was published in the Journal of Nano medicine showed that a liposomal formulation improved with the herbal extract Artemisia annua might effectively prevent malaria. (42)

CASE STUDIES AND REAL-WORLD APPLICATIONS

CASE STUDY 1: HERBAL ANTI- CANCER NANO FORMULATIONS

The anti-cancer properties of curcumin, a compound derived from turmeric that was nano-formulated, were investigated using artificial intelligence. The AI model found synergistic interactions between several phytochemicals, which enhanced curcumin's bioavailability and anti-cancer efficacy. (43)

CASE STUDY 2: IMPROVING BIOAVAILABILITY WITH AI

The research emphasises the application of artificial intelligence aiming to boost the bioavailability of nano-encapsulated ginseng extract. The study identified the most advantageous nanoparticle composition by using optimisation algorithms, which led to a fourfold improvement in bioavailability when compared to conventional techniques. (44)

ADVANTAGES OF AI NANO-HERBAL FORMULATIONS

Compared against conventional herbal remedies, nano-herbal composition have a number of advantages. These advantages cover a range of delivery and efficacy factors.

1. IMPROVED SOLUBILITY AND BIOAVAILABILITY:

Research shows that nano formulations can greatly improve the solubility and bioavailability of herbal extracts, resulting in a decrease in possible toxicity and an increase in therapeutic efficiency. (45)

2. TARGETED DELIVERY:

The creation of nano-herbal formulations makes it possible to precisely target particular anatomical regions, increasing the effectiveness of treatment while lowering the possibility of side effects. (46)

3. IMPROVED STABILITY:

By drastically lowering oxidation and degradation rates, nano-herbal formulations increase the longevity of herbal remedies. Additionally, the danger of toxicity and unfavourable side effects that are frequently connected with conventional herbal medicines may be reduced by these nano-encapsulated herbal drugs. (47)

4. IMPROVED EFFICACY:

Clinical trial data can be continually monitored by artificial intelligence (AI), which helps with early safety problem detection and real-time efficacy validation. AI can also significantly enhance the formulation and design of nano herbal medications, increasing their efficacy and decreasing their toxicity. Additionally, using AI to automate different processes involved in the development and production of these formulations might boost output and lower overall expenses. (48)

5. ENHANCED SAFETY:

By spotting any negative effects of nano-formulations before they are clinically tested, artificial intelligence simulations and predictive modelling techniques might enhance safety measures. (49). By spotting potential safety issues with nano herbal medicine mixtures, artificial intelligence (AI) can lessen the possibility of negative reactions. (50).

6. PERSONALIZED THERAPIES:

The merging of artificial intelligence with nano-herbal medicine offers a significant opportunity for enhancing customised treatment methods. By analysing vast amounts of patient data, such as genetic information, medical histories, and lifestyle factors, artificial intelligence (AI) can help tailor nano botanical medicines to each patient's unique needs. This customised strategy minimises adverse effects, maximises therapeutic benefits, and makes it easier to administer the safest and the most effective treatments. Artificial intelligence can also aid in the development of personalised nano-herbal drugs that are suited to each patient's specific needs and characteristics. (51).

7. COMBINING CONVENTIONAL WISDOM WITH CONTEMPORARY SCIENCE

By making it easier to combine traditional herbal methods with novel scientific study, artificial intelligence has considerably to offer the field of nano herbal medicine. By analysing large datasets from traditional medicine, AI can identify potent herbal combinations and support their scientific validation. This integration increases the acceptance of herbal medicines in modern medicine while preserving the richness of cultural history.(52)

8. BETTER DELIVERY AND FORMULATION SYSTEMS

The solubility, stability, and bioavailability of herbal substances are greatly improved by nanotechnology. AI can also enhance these nano formulations by predicting their biological performance, modelling interactions, and identifying the most effective delivery strategies. This is essential for creating tailored therapies that maximise therapeutic advantages while minimising negative effects. (53)

9. DRUG DISCOVERY AND DEVELOPMENT

AI algorithms are faster and more effective than conventional methods for analysing the pharmacological characteristics, biological activities, and chemical structures of herbal compounds. For example, by analysing the molecular fingerprints of nano-formulated herbal constituents, machine learning models can precisely predict their activity, which significantly reduces the time and expense associated with medication discovery. This method simplifies the entire testing process in addition to identifying promising candidates for additional development(54)

APPLICATION:

- ✓ The development of innovative, adaptable, patient-focused nanomedicines has also benefited from the use of generative AI. To characterise the intratumoral distribution of quantum dots following injection, for instance, Tang and associates created a Generative Adversarial Network for Distribution Analysis (GANDA). (55)
- ✓ The In order to provide images with the same spatial resolution with the least amount of loss and dependability, the model was developed utilising tumour vasculature and cell nuclei taken from whole-slide images of breast cancer sections. The surface properties of NPs have a major impact on their biological behaviour, including protein corona formation and opsonisation, which impacts their therapeutic efficacy. Protein corona formation can be influenced by a wide range of quantitative and qualitative parameters, making it difficult to forecast using density functional theory or a basic linear regression model. A recent study combined machine learning and meta-analysis to create a model. (56)
- ✓ Offering a practical way to forecast the functional composition of the protein corona and the identification of NPs by cells. In order to evaluate liver/spleen accumulation from protein adsorption on NPs and forecast their in vivo behaviour, Lazarovits et al. (57).developed a supervised DNN model using experimental proteomics data of NPs. In order to create NPs with high drug loading and/or deliver medications to certain cells for a variety of therapeutic uses, researchers have also used machine learning algorithms. (58)
- ✓ Predicting and optimising safety profiles is another use of AI/ML that can greatly lower the dangers associated with translating nanomedicine. In order to forecast immunogenicity or tolerance, for instance, these techniques are utilised to analyse vast amounts of bioanalytical data derived from the characterisation of biomarkers (such as anti-drug antibodies) from patient samples. (59)
- ✓ Because AI-driven technologies, such deep learning techniques, can analyse huge unstructured data, they have advanced nanomedicine manufacturing and quality control. tured data and how much more predictable they are than conventional techniques. The majority of applications documented in the literature concentrated on formulation development, process optimisation, quality control using process analytical technology (PAT), and identifying critical quality attributes (CQAs) and critical process parameters (CPPs). In order to logically construct liposomes with an optimal particle size and polydispersity index (PDI), Rebollo et al. used artificial neural networks (ANNs) and design of experiments (DoE) to determine crucial formulation and process parameters.(60)
- ✓ The field of continuous manufacturing has also seen an increase in the use of AI and ML tools. In pharmaceutical continuous production, the PAT initiative seeks to Using in-line, at-line, and online sensors, real-time measurements of CQAs and CPPs allow for mistake correction and prevention, process condition adjustment to avert a failed batch, and eventually an agile manufacturing paradigm. Real-time monitoring of product CQAs and contaminants is made possible by PAT instruments like Raman and near-infrared spectroscopy, which improves manufacturing process and product quality control. A significant amount of data with multiple variables is produced when PAT and continuous production are integrated. In this sense, ML-based methods like ANNs, which are naturally adaptable, able to modify model behaviour for ongoing performance enhancement, and capable of real-time large data analysis, enabling autonomous decision-making, adaptive control, and the development of digital twins and smart factories .(61)

CONCLUSION

The combination of artificial intelligence with nano-herbal medicine has made it possible to improve the efficacy, accuracy, and customisation of therapies made from natural plants. The discipline of nano herbal medicine is positioned to provide more efficient and individualised treatments for a variety of medical ailments by utilising AI's strengths in rational design, targeted delivery, predictive modelling, and quality assurance. It is critical to overcome the obstacles and fully utilise this technology's transformative potential to enhance human health as advancements in this field continue. Combining AI with nano-herbal medicine has many advantages, including improvements in formulation, drug discovery, personalised therapies, predictive analytics, quality control, and the fusion of traditional and contemporary knowledge. All stakeholders, including academics, medical professionals, and politicians, will need to make full use of these tools as research in this field advances. Future studies should focus on how these developments will affect patient outcomes and the healthcare system overall in the long run.

DISCUSSION

The ethical and legal issues surrounding the use of AI in nano-herbal medicine are also examined in this review. AI has emerged as a key technology in this area, helping in formulation development optimisation, bioactivity prediction, and the analysis of massive datasets. All stakeholders, including researchers, medical professionals, and legislators, must adopt these technologies as this field of study develops in order to optimise their advantages. The long-term effects of these advances on patient outcomes and the healthcare system as a whole should be the focus of future research.

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